

Learned Discourses

setac@setac.org

Timely Scientific Opinions

Intent. The intent of Learned Discourses is to provide a forum for open discussion by and for SETAC members. These articles reflect the professional opinions of the authors regarding scientific issues. They do not represent SETAC positions or policies. And, although they are subject to editorial review for clarity, consistency, and brevity, these articles are not peer reviewed.

The Learned Discourses date from 1996 in the North America *SETAC News*; however, their continued success depends on our contributors. We encourage timely submissions that will inform and stimulate discussion. We expect that many of the articles will address controversial topics, and we promise to give dissenting opinions a chance to be heard. If you disagree with an opinion expressed here, don't complain—submit a reply!

Rules. All submissions must be succinct: no longer than 1000 words, no more than 6 references, and at most one table or figure. Reference format must follow that of the journal *Environmental Toxicology and Chemistry* except that text citations are by author and date, rather than numeric. Topics must fall within SETAC's sphere of interest. And, most importantly, respect and courtesy must prevail; personal attacks and other unprofessional behavior will not be tolerated.

Submissions. Send submissions as email attachments to Peter Chapman (pchapman@attglobal.net).

In a Nutshell...

ENVIRONMENTAL CHEMISTRY

Bioaccumulation Reality Check

F. Gobas, M. Moore, J. Hermens, J. Arnot

Be cautious when assessing bioaccumulation of high K_{ow} high MW chemicals

RISK ASSESSMENT

Probabilistic Risk Assessment of Pesticides: Is It Working?

J. Giddings, W. Warren-Hicks

Benefits and drawbacks are summarized from various stakeholder viewpoints

Fragrance materials and the environment - is there a risk?

D. Salvito, R. Senna, C. McIntosh

Past and continuing efforts to answer this question are outlined

ECOTOXICOLOGY

Ecotoxicology of Nanoparticles (NPs)

T. Fernandes, P. Rosenkranz, A. Ford, N. Christofi, V. Stone

Although preparation artifacts render previous studies suspect, concerns remain

Learned Discourses Editor

Peter M. Chapman
Golder Associates Ltd.
195 Pemberton Avenue
North Vancouver, BC V7P 2R4
Canada
T 1-604-904-4005
F 1-604-662-8548
pmchapman@golder.com



APPLIED SCIENCE

Science and Politics: SETAC and the 'Untreated Sewage' Issue in Western Canada

P.M. Chapman

A report not provided, a political decision made then overruled, future environmental initiatives in doubt

Public View: Benefits. Advocates and critics of PRA agreed that the public perceives little benefit in PRA of pesticides. However, to an objective public stakeholder, PRA can provide a more realistic estimate of risk. PRA also allows more informed comparison of risks and benefits, so public funds can be applied to the most pressing issues and not wasted on activities that do little to reduce actual risk.

Public View: Drawbacks. PRA is difficult to understand and interpret. The public is suspicious about statistics and ignorant about probability. PRA is seen as enabling more “lenient” decisions rather than greater environmental protection. PRA also demonstrates that risk is rarely zero, a fact that makes many people uncomfortable.

Although we included individuals from all three of SETAC’s traditional sectors in our informal survey, most of the replies summarized above came from industry and academia. Although the EPA is developing PRA methods for pesticides (U.S. EPA 2004), the Agency’s perspective on PRA has not often been articulated. For insight, we turned to a recent review by EPA of one of our own PRAs submitted in support of a product registration. From the review, we extracted comments that revealed, by implication, elements EPA considers important in a pesticide PRA. What we found is summarized below:

Scope. The PRA should address all issues of regulatory concern. The temporal and spatial scale must be appropriate, and spatial and temporal variability must be considered. Surrogate species used in the analysis must represent all the species of concern.

Model. The risk model used in the PRA must adequately represent the assessment scenario, and must account for all factors that affect exposure and effects. Toxicokinetics must be accurately simulated. Input variables must be selected carefully, and their range must represent all scenarios of interest.

Assumptions. Model assumptions must be plausible and supported by reference to published research. Assumptions about distributions must be justified. The sensitivity of the model to the assumptions should be explored. The assumptions should not limit the range of predicted outcomes.

Data. The data used in the PRA must be complete and consistent. Data quality must meet EPA standards. All relevant data should be incorporated into the model. The data must represent the situations being assessed.

Uncertainties. A quantitative uncertainty analysis is needed. Uncertainties stemming from assumptions must be clearly presented. Risk often depends on local conditions that are difficult to quantify on a national scale; depending on the assumptions used, risk could range from minimal to high. Bayesian approaches are “innovative and creative” but their limitations are unknown to the Agency.

Risk Characterization. The PRA should not understate the risk. Model predictions should be compared with field observations of effects.

In this particular case, EPA concluded that the PRA was insufficient to alter the conclusions reached by previous deterministic assessments. Given the regulatory outcome, did this PRA “work”? In our view, and the view of the companies that sponsored the assessment, the answer is “yes.” Most of EPA’s concerns can be addressed, without altering the model or the

approach, by correcting misunderstandings, modifying data selection, and extending the scope to other species and scenarios. More importantly, the PRA resulted in a better understanding of the sources of uncertainty affecting the risk estimation. Discussion can now focus on assumptions that most affected the outcome, and additional data can be sought to address those assumptions.

References

U.S. EPA. 2004. A discussion with the FIFRA Scientific Advisory Panel regarding the terrestrial and aquatic Level II refined risk assessment models (Version 2.0). U.S. Environmental Protection Agency, Office of Pesticide Programs, Washington, DC. <http://www.epa.gov/scipoly/sap/meetings/2004/index.htm#march>.

Fragrance materials and the environment - is there a risk?

Daniel Salvito¹, Ronald Senna^{2,3}, Colin McIntosh⁴
¹*Research Institute for Fragrance Materials, Woodcliff Lake, NJ, USA,* ²*International Flavors and Fragrances Inc., Shrewsbury, NJ, USA,* ³*International Fragrance Association, Brussels, Belgium,* ⁴*Firmenich Inc, Princeton, NJ, USA,* <dsalvito@rifm.org>

Introduction

Over the past decade, there has been increasing interest among the academic, regulatory, and NGO communities concerning the environmental “risk” from non-traditional chemicals. These are chemicals that have not traditionally been used as the basis for our understanding of environmental “risk” and thus for the implementation of regulatory frameworks compared to substances such as pesticides, PCBs, and PAHs. Multiple terms are used to identify these chemicals: emerging pollutants and pharmaceutical and personal care products (PPCPs) are two examples of new nomenclature applied to some of these chemicals.

Many of these chemicals used today in commerce are neither “new” nor “emerging”. They have been used for decades in a variety of consumer products and other industrial applications with no known adverse effects. Quite understandably, however, as it would appear that there is a dearth of environmental fate and effects information on these chemicals, questions arise as to their potential to incur a risk to the environment.

As fragrance materials are often cited as “emerging pollutants” or PPCPs, it is the intent of this Learned Discourse to outline our present understanding about these materials and their potential to affect the environment.

What are Fragrance Materials?

Typically, fragrance ingredients consist of organic molecules of low molecular weight (<300 mu) with vapor pressures less than 2 mm Hg. These chemicals represent a wide variety of chemical classes including esters, acids, aldehydes, ketones, etc. of varying physical-chemical properties. While the majority of these materials are used at very low commercial volumes; a few are higher tonnage materials. Fragrance materials consist of mixtures of these ingredients and can range from ten to several

hundred individual ingredients, depending on the application (e.g., perfumes, soaps and detergents, cosmetics and other consumer products).

Currently available information

The nitromusk and polycyclic musk compounds are some of the most studied chemicals within the fragrance industry. These materials are often listed as PPCPs and, although they represent two different structural classes, are often collectively referred to as “musk”. There are over 40 peer-reviewed publications on the nitromusks and 50 on the polycyclic musks, and the list continues to grow. Their risk assessments are currently under review by the European Union. Thus far, the European Chemicals Bureau has concluded that the polycyclic musks HHCb (1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta- γ -2-benzopyran) and AHTN (6-acetyl-1,1,2,4,4,7-hexamethyltetraline) are not PBT (Persistent, Bioaccumulative, Toxic) substances, and the European Scientific Committee for Cosmetics and Non-Food Products has affirmed their continued safe use in consumer products (SCCNFP 2002a, SCCNFP 2002b). A recent summary of the environmental risk assessments of these materials is available in HERA (2004).

The difficulty arises within the literature and the popular press when the “discovery” of these chemicals in the environment is separated from an assessment of their potential risk; i.e., comparison to known, measured effects. While we acknowledge the great advances in analytical chemistry that have enabled us to find chemicals in the environment at ever decreasing concentrations, we encourage the comparison of these analytical measurements with the reported effects of the chemical in a risk assessment context. This context would further benefit from more thorough reviews of the existing literature and searches of regulatory databases for risk-based information. Identification and quantification is not risk assessment.

Risk assessment and fragrance materials

The fragrance material industry, through its non-profit research institute, the Research Institute for Fragrance Materials (RIFM), published an aquatic screening level risk assessment paradigm (Salvito et al. 2002) to establish research and testing priorities for over 2,000 discrete, organic chemicals used in fragrance compounds. The aquatic scenario is a reasonable worst case, because the major route of exposure for fragrance ingredients is in down-the-drain products. This screening tool provides for multiple tiers of assessment beginning with basic physical-chemical properties (molecular weight, octanol-water partitioning coefficient, and regional volume of use) and a quantitative structure-activity relationship to determine aquatic toxicity (applying a large application factor to determine the Predicted No-Effect Concentration), and ends with the input of available, measured data to establish a set of materials for further testing, if necessary.

This screening level assessment is revised with each new volume of use survey performed by the fragrance industry (minimally every five years) and as new fate and effects data become available. The initial screening resulted in greater than 92% of the materials being found to have an aquatic risk quotient less than 1 (minimal risk). Through the use of structure-activity groups and read-across, and data that have been generated as

a result of regulatory programs and industry sponsored studies, this set of priority materials has been continuously reduced.

Fragrance materials and the environment

Clearly, an aquatic screening level assessment does not answer all the questions that may arise regarding these materials and the environment. The fragrance material industry, through RIFM, has funded research in the areas of soil fate, biotransformation, and, presently, bioavailability from sediment exposures. Other research groups have looked at the atmospheric chemistry of key fragrance ingredients and the potential for endocrine effects. Monitoring of these materials in various environmental compartments and biota is also on-going. A broader review of the issue of fragrance material use and their potential environmental impact is provided by Salvito et al. (2004).

While more data are always desired, the existing information available, and considering current use levels, indicates that fragrance materials present a minimal environmental risk. The fragrance industry has voluntarily committed to continue to study these materials in various environmental compartments and publish their findings in the peer-reviewed literature. The issue as to whether or not fragrance materials pose a risk to the environment has not yet been fully answered, but data available to date would argue against it.

References

- SCCNFP. 2002a. Opinion of the Scientific Committee on Cosmetic Products and Non-Food Products Intended for Consumers Concerning 6-Acetyl-1,1,2,4,4,7-Hexamethyltetraline (AHTN). SCCNFP/0609/02
- SCCNFP. 2002b. Opinion of the Scientific Committee on Cosmetic Products and Non-Food Products Intended for Consumers Concerning Hexahydro-Hexamethyl-Cyclopenta (γ)-2-Benzopyran (HHCb). SCCNFP/0610/02
- HERA, 2004. Human and Environmental Risk Assessment on Ingredients of Household Cleaning Products: Polycyclic musks AHTN (CAS 1506-02-1) and HHCb (CAS 1222-05-05) Environmental Section Ver. 2.0 (<http://www.heraproject.com/RiskAssessment.cfm>)
- Salvito DT, Senna RJ, Federle TW. 2002. A Framework for prioritizing fragrance materials for aquatic risk assessment. *Environ Toxicol Chem* 21: 1301-1308.
- Salvito DT, Vey MGH, Senna RJ. 2004. Fragrance materials and their environmental impact. *Flav Frag J* 19:105-108.

Ecotoxicology of Nanoparticles (NPs)

T. F. Fernandes, P. Rosenkranz, A. Ford, N. Christofi, and V. Stone

Napier University, Edinburgh, UK,
[<t.fernandes@napier.ac.uk>](mailto:t.fernandes@napier.ac.uk)

Introduction

Nanotechnology is a rapidly developing field of science, technology and innovation. It involves the development and manufacture of materials in the nanometer size range and includes the production and use of nanoparticles (NPs; particles with at least one dimension of less than 100 nm). Due to their small size a relatively large proportion of the atoms and molecules making up the particles are exposed at the particle surface